



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:52 PM GMT

PDB ID : 4Q6F
Title : Crystal structure of human BAZ2A PHD zinc finger in complex with unmodified H3K4 histone peptide
Authors : Tallant, C.; Overvoorde, L.; Krojer, T.; Filippakopoulos, P.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Ciulli, A.; Knapp, S.; Structural Genomics Consortium (SGC)
Deposited on : 2014-04-22
Resolution : 1.91 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

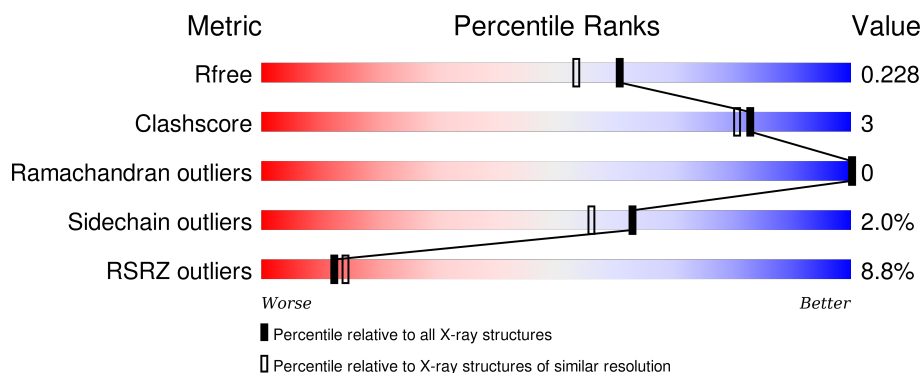
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	5832 (1.94-1.90)
Clashscore	102246	6540 (1.94-1.90)
Ramachandran outliers	100387	6464 (1.94-1.90)
Sidechain outliers	100360	6465 (1.94-1.90)
RSRZ outliers	91569	5846 (1.94-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	58	<div> <div>5%</div> <div>91%</div> <div>5%</div> </div>
1	B	58	<div> <div>7%</div> <div>78%</div> <div>14%</div> <div>7%</div> </div>
1	C	58	<div> <div>5%</div> <div>81%</div> <div>7%</div> <div>12%</div> </div>
1	D	58	<div> <div>2%</div> <div>81%</div> <div>10%</div> <div>9%</div> </div>
2	F	5	<div> <div>60%</div> <div>80%</div> <div>20%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	5	
2	H	5	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	A	1803	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 1868 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Bromodomain adjacent to zinc finger domain protein 2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	56	Total	C	N	O	S	0	0	0
			432	266	76	81	9			
1	B	54	Total	C	N	O	S	0	0	0
			423	261	75	78	9			
1	C	51	Total	C	N	O	S	0	0	0
			394	244	69	72	9			
1	D	53	Total	C	N	O	S	0	0	0
			415	257	73	76	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1671	HIS	-	EXPRESSION TAG	UNP Q9UIF9
A	1672	MET	-	EXPRESSION TAG	UNP Q9UIF9
B	1671	HIS	-	EXPRESSION TAG	UNP Q9UIF9
B	1672	MET	-	EXPRESSION TAG	UNP Q9UIF9
C	1671	HIS	-	EXPRESSION TAG	UNP Q9UIF9
C	1672	MET	-	EXPRESSION TAG	UNP Q9UIF9
D	1671	HIS	-	EXPRESSION TAG	UNP Q9UIF9
D	1672	MET	-	EXPRESSION TAG	UNP Q9UIF9

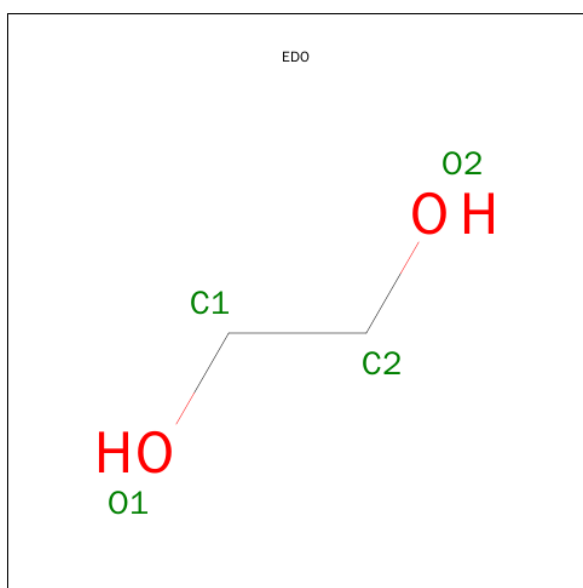
- Molecule 2 is a protein called unmodified H3K4 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	5	Total	C	N	O	0	0	0
			41	24	10	7			
2	G	5	Total	C	N	O	0	0	0
			41	24	10	7			
2	H	4	Total	C	N	O	0	0	0
			32	19	8	5			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	Zn 2	0	0
3	A	2	Total 2	Zn 2	0	0
3	D	2	Total 2	Zn 2	0	0
3	C	2	Total 2	Zn 2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total 20	O 20	0	0
5	B	18	Total 18	O 18	0	0
5	C	7	Total 7	O 7	0	0

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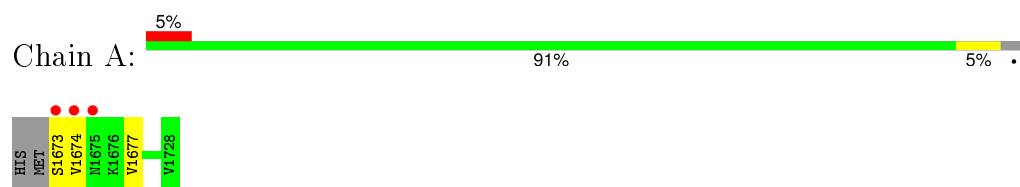
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	23	Total	O	0	0
			23	23		
5	F	2	Total	O	0	0
			2	2		

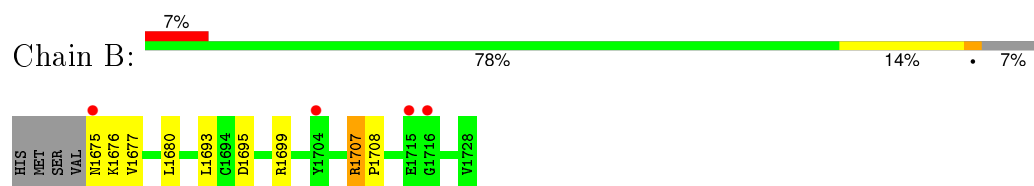
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

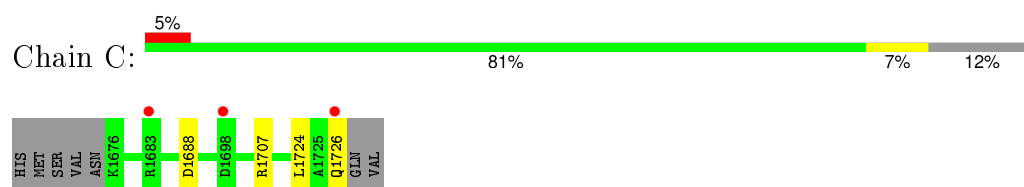
- Molecule 1: Bromodomain adjacent to zinc finger domain protein 2A



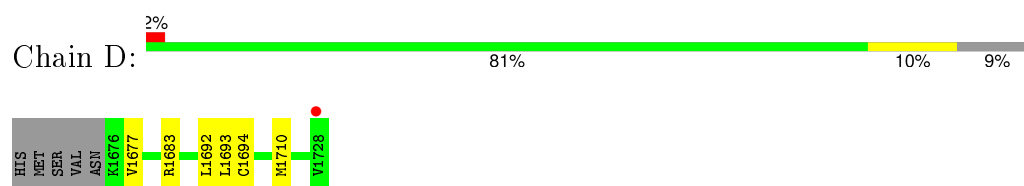
- Molecule 1: Bromodomain adjacent to zinc finger domain protein 2A



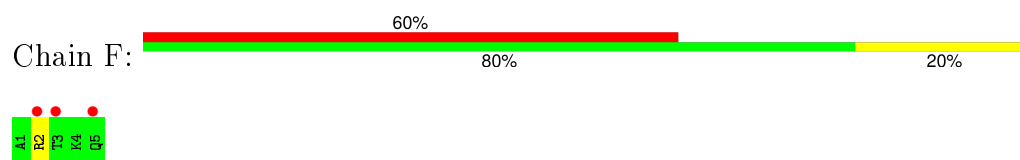
- Molecule 1: Bromodomain adjacent to zinc finger domain protein 2A



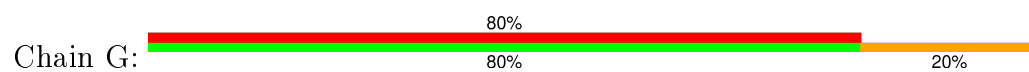
- Molecule 1: Bromodomain adjacent to zinc finger domain protein 2A



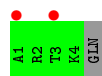
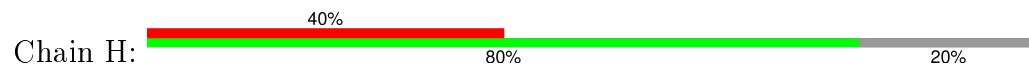
- Molecule 2: unmodified H3K4 peptide



- Molecule 2: unmodified H3K4 peptide



- Molecule 2: unmodified H3K4 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	71.87Å 71.87Å 98.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.06 – 1.91 29.06 – 1.91	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.06-1.91) 99.8 (29.06-1.91)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 1.92Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.183 , 0.219 0.189 , 0.228	Depositor DCC
R_{free} test set	1002 reflections (5.14%)	DCC
Wilson B-factor (Å ²)	27.8	Xtrriage
Anisotropy	0.028	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 37.4	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Outliers	0 of 20508 reflections	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1868	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.64 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.4790e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	0/440	0.80	0/594
1	B	0.59	0/431	0.84	1/580 (0.2%)
1	C	0.52	0/402	0.83	2/543 (0.4%)
1	D	0.67	0/423	0.80	1/569 (0.2%)
2	F	0.65	0/40	0.88	0/51
2	G	0.55	0/40	1.05	0/51
2	H	0.52	0/31	0.77	0/39
All	All	0.60	0/1807	0.82	4/2427 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1683	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	B	1707	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	C	1707	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	C	1707	ARG	NE-CZ-NH2	-5.28	117.66	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1673	SER	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	432	0	400	1	0
1	B	423	0	397	6	0
1	C	394	0	363	1	0
1	D	415	0	391	3	0
2	F	41	0	48	0	0
2	G	41	0	48	1	0
2	H	32	0	40	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
4	D	4	0	6	0	0
5	A	20	0	0	0	0
5	B	18	0	0	1	0
5	C	7	0	0	0	0
5	D	23	0	0	1	0
5	F	2	0	0	0	0
All	All	1868	0	1705	11	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (11) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1674:VAL:O	1:A:1677:VAL:HG12	1.98	0.63
1:B:1677:VAL:HG21	1:B:1693:LEU:HD22	1.84	0.60
1:B:1677:VAL:HG21	1:B:1693:LEU:CD2	2.36	0.55
5:B:1915:HOH:O	1:C:1724:LEU:HD12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1675:ASN:HB2	1:B:1676:LYS:HA	1.93	0.50
1:D:1694:CYS:O	5:D:1916:HOH:O	2.20	0.49
1:D:1677:VAL:HG21	1:D:1693:LEU:HD22	1.96	0.47
1:B:1680:LEU:HD21	1:B:1699:ARG:HD3	2.00	0.44
1:B:1707:ARG:HA	1:B:1708:PRO:C	2.40	0.41
1:D:1692:LEU:HD11	1:D:1710:MET:CE	2.51	0.41
1:B:1695:ASP:OD1	2:G:2:ARG:NH1	2.54	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	54/58 (93%)	53 (98%)	1 (2%)	0	100	100
1	B	52/58 (90%)	52 (100%)	0	0	100	100
1	C	49/58 (84%)	48 (98%)	1 (2%)	0	100	100
1	D	51/58 (88%)	51 (100%)	0	0	100	100
2	F	3/5 (60%)	3 (100%)	0	0	100	100
2	G	3/5 (60%)	3 (100%)	0	0	100	100
2	H	2/5 (40%)	2 (100%)	0	0	100	100
All	All	214/247 (87%)	212 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	49/52 (94%)	49 (100%)	0	100	100
1	B	48/52 (92%)	48 (100%)	0	100	100
1	C	44/52 (85%)	42 (96%)	2 (4%)	34	21
1	D	47/52 (90%)	47 (100%)	0	100	100
2	F	4/4 (100%)	3 (75%)	1 (25%)	1	0
2	G	4/4 (100%)	3 (75%)	1 (25%)	1	0
2	H	3/4 (75%)	3 (100%)	0	100	100
All	All	199/220 (90%)	195 (98%)	4 (2%)	63	56

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1688	ASP
1	C	1726	GLN
2	F	2	ARG
2	G	2	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1687	ASN
1	B	1675	ASN
1	B	1687	ASN
1	C	1687	ASN
1	D	1687	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	A	1803	-	3,3,3	0.57	0	2,2,2	0.08	0
4	EDO	B	1803	-	3,3,3	0.27	0	2,2,2	0.55	0
4	EDO	D	1803	-	3,3,3	0.52	0	2,2,2	0.06	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	1803	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1803	-	-	0/1/1/1	0/0/0/0
4	EDO	D	1803	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	56/58 (96%)	0.54	3 (5%) 29 33	21, 32, 55, 72	0
1	B	54/58 (93%)	0.41	4 (7%) 17 20	22, 30, 53, 76	0
1	C	51/58 (87%)	0.57	3 (5%) 26 29	23, 40, 62, 73	0
1	D	53/58 (91%)	0.46	1 (1%) 70 73	21, 29, 49, 53	0
2	F	5/5 (100%)	1.93	3 (60%) 0 0	38, 39, 53, 55	0
2	G	5/5 (100%)	3.94	4 (80%) 0 0	53, 56, 65, 81	0
2	H	4/5 (80%)	2.13	2 (50%) 0 0	54, 56, 59, 67	0
All	All	228/247 (92%)	0.63	20 (8%) 12 14	21, 34, 62, 81	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	5	GLN	8.1
1	A	1674	VAL	7.7
1	A	1675	ASN	5.0
2	G	2	ARG	4.9
1	D	1728	VAL	4.3
1	B	1675	ASN	4.0
1	A	1673	SER	3.8
1	C	1698	ASP	3.6
1	C	1726	GLN	3.2
1	C	1683	ARG	3.1
2	G	1	ALA	3.1
1	B	1715	GLU	3.0
2	F	5	GLN	3.0
2	F	3	THR	2.9
2	H	3	THR	2.6
2	H	1	ALA	2.4
2	G	3	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	1716	GLY	2.3
1	B	1704	TYR	2.1
2	F	2	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	EDO	A	1803	4/4	0.95	0.17	4.14	40,45,46,47	0
4	EDO	B	1803	4/4	0.92	0.13	0.73	49,52,52,57	0
3	ZN	A	1801	1/1	1.00	0.10	-0.44	26,26,26,26	0
3	ZN	B	1801	1/1	0.99	0.12	-0.48	26,26,26,26	0
4	EDO	D	1803	4/4	0.95	0.13	-0.55	32,38,40,43	0
3	ZN	D	1802	1/1	1.00	0.07	-0.67	21,21,21,21	0
3	ZN	D	1801	1/1	1.00	0.10	-0.96	23,23,23,23	0
3	ZN	B	1802	1/1	1.00	0.07	-0.99	24,24,24,24	0
3	ZN	C	1800	1/1	0.99	0.08	-1.54	32,32,32,32	0
3	ZN	C	1801	1/1	1.00	0.07	-1.73	35,35,35,35	0
3	ZN	A	1802	1/1	0.99	0.07	-2.17	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.